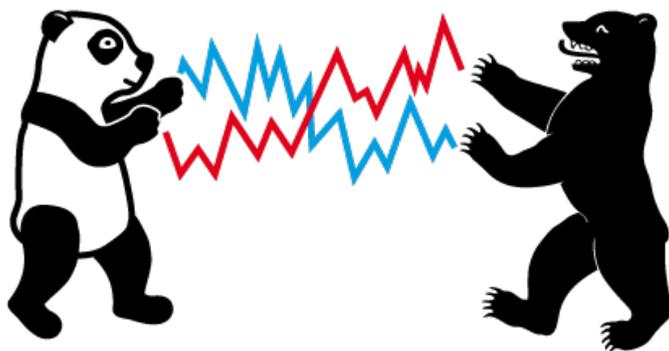




# Gaussian Process Forecast with multidimensional distributional entries

Francois Bachoc <sup>\*</sup>  
Alexandra Suvorikova <sup>\*2</sup>  
Jean-Michel Loubes <sup>\*</sup>  
Vladimir Spokoiny <sup>\*2</sup>



<sup>\*</sup> Institut de Mathematiques de Toulouse, France  
<sup>\*2</sup> WIAS, Germany

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# Gaussian Process Forecast with multidimensional distributional entries

**Francois Bachoc**

*Institut de Mathématiques de Toulouse*

FRANCOIS.BACHOC@MATH.UNIV-TOULOUSE.FR

**Alexandra Suvorikova**

*Weierstrass Institute for Applied Analysis and Stochastics*

ALEXANDRA.SUVORIKOVA@WIAS-BERLIN.DE

**Jean-Michel Loubes**

*Institut de Mathématiques de Toulouse*

LOUBES@MATH.UNIV-TOULOUSE.FR

**Vladimir Spokoiny**

*Weierstrass Institute for Applied Analysis and Stochastics*

VLADIMIR.SPOKOINY@WIAS-BERLIN.DE

## Abstract

In this work, we propose to define Gaussian Processes indexed by multidimensional distributions. In the framework where the distributions can be modeled as i.i.d realizations of a measure on the set of distributions, we prove that the kernel defined as the quadratic distance between the transportation maps, that transport each distribution to the barycenter of the distributions, provides a valid covariance function. In this framework, we study the asymptotic properties of this process, proving micro ergodicity of the parameters.

**Keywords:** Gaussian Process, Kernel methods, Wasserstein Distance.

## 1. Introduction

Gaussian process models rely on the definition of a covariance function that characterises the correlations between values of the process at different observation points. As the notion of similarity between data points is crucial, *i.e.* close location inputs are likely to have similar target values, covariance functions, or kernels, are the key ingredient in using Gaussian processes, since they define nearness or similarity.

In this paper we propose to define Gaussian processes indexed on distributions on  $\mathbb{R}^d$ . This situation happens for instance in numerical code experiments when the prior knowledge of the process may not be an exact value but rather a set of acceptable values that will be modeled using a prior distribution. Hence we observe output values for such probability distributions and want to forecast the process for other ones. This requires defining proper covariance functions indexed on the set of distributions. There has been a huge amount of literature dealing with the use of Gaussian Processes in Machine Learning over the last decade. We refer for instance to ?, ? or ? and references therein.

The simplest method is to compare a set of parametric features built from the probability distributions, such as the mean or the higher moments. This approach is limited as the effect of such parameters do not take into account the whole shape of the law. Specific kernel should be designed in order to map distributions into a reproducing kernel Hilbert space in which the whole arsenal of kernel methods can be extended to probability measures. This issue has recently been considered in

? or ?. We aim at basing these kernels on the Wasserstein, or transport-based, distance which was shown to be relevant and insightful for comparing distributions. This work has been studied for one dimensional case in ? using the special expression of Wasserstein distance in dimension 1. Yet this case hides the difficulty of the problem by using the optimal coupling with the uniform random variable. In the general dimension case, in order to build a valid kernel from the Wasserstein distance, we restrict ourselves to the case where the distributions are drawn following a common distribution  $\mathbb{P}$  over the set of distributions with finite second order moment. This enables to define a notion of Fréchet mean (or barycenter) of the distributions, which will be used to compare the distributions between themselves. Actually, we use this barycenter to construct a covariance by considering the transportation maps from the distributions to this barycenter and using the distance between these maps as a way to generate kernels. The notion of Wasserstein barycenters and their use in machine learning and in statistics is a growing research field. We mention for instance ?, ?, ? for instance.

We thus obtain a Gaussian process indexed by distributions that belong to the support of  $\mathbb{P}$ . We then provide asymptotic results on the estimation of parameters of covariance functions constructed as described above, as the number of observed values of the process increases. Since the process is observed for input distributions belonging to the (fixed) support of  $\mathbb{P}$ , we provide infill asymptotic results ?. More precisely, we show a very general result for the microergodicity of covariance parameters. We mention that for the same purpose, another point of view is to consider a distribution regression framework described in ?.

The paper falls into the following parts. In Section 2 we recall some definitions on kernels and on the notion of Wasserstein barycenter of distributions. Section 3 is devoted to the construction and analysis of an appropriate kernel for probability measures on  $\mathbb{R}^d$  for  $d \geq 1$ . Asymptotic results and micro-ergodicity of the parameters are presented in Section 4. Section 5 is devoted to numerical applications while the proofs are postponed to the appendix.

## 2. Gaussian Processes indexed by distributions

### 2.1. Framework of the study

Gaussian process models are now widely used in fields such as geostatistics, computer experiments or machine learning ?, ?. A Gaussian process model consists in modeling an unknown function as a realization of a Gaussian process, and hence corresponds to a functional Bayesian framework. For instance, in computer experiments, the input points of the function are simulation parameters and the output values are quantities of interest obtained from the simulations.

In this paper we focus on Gaussian processes for which the input parameters are in  $\mathcal{P}(\mathbb{R}^p)$  the set of distributions over  $\mathbb{R}^p$ . To study such models, Gaussian Processes must be defined over the set of distributions.

Let us recall that a Gaussian process  $(Y_x)_{x \in E}$  indexed by a set  $E$  is entirely characterised by its mean and covariance functions. Its covariance function is defined by  $(x, y) \in E^2 \rightarrow \text{Cov}(X_x, X_y)$ . A function  $K : E \times E \mapsto \mathbb{R}$  is actually the covariance of a random process if and only if it is a *positive definite kernel*, that is to say for every  $x_1, \dots, x_n \in E$  and  $\lambda_1, \dots, \lambda_n \in \mathbb{R}$ ,

$$\sum_{i,j=1}^n \lambda_i \lambda_j K(x_i, x_j) \geq 0. \tag{1}$$

In this case we say that  $K$  is a *covariance kernel*. We also say that  $K$  is a *negative definite kernel* if the quadratic form in (1) is non-positive when  $\sum_{i=1}^n \lambda_i = 0$ . Hence we need to build a function on  $\mathcal{P}(\mathbb{R}^p) \times \mathcal{P}(\mathbb{R}^p)$  which satisfies the positive constraint (1).

It is then desirable that the covariance function evaluated at  $(\mu, \nu) \in \mathcal{P}(\mathbb{R}^p)^2$  be related to the Wasserstein distance between  $\mu$  and  $\nu$  (see ?). In the one dimensional case, this has been proved to be possible in ?. Indeed, in this case, using a covariance based on the Wasserstein distance amounts to using the well-known optimal coupling (see ?) for all  $\mu \in \mathcal{P}(\mathbb{R})$  with finite second order moments

$$Z_\mu := F_\mu^{-1}(U), \quad (2)$$

where  $F_\mu^{-1}$  is defined as

$$F_\mu^{-1}(t) = \inf\{u, F_\mu(u) \geq t\},$$

and denotes the quantile function of the distribution  $\mu$  and where  $U$  is an uniform random variable. This coupling can be seen as a non-Gaussian random field indexed by the set of distributions on the real line with finite second order moments. As such, its variogram

$$(\mu, \nu) \mapsto \mathbb{E}(Z_\mu - Z_\nu)^2 \quad (3)$$

defines a negative definite kernel, equal to  $W_2^2(\mu, \nu)$  since the coupling  $(Z_\mu)$  is optimal. This kernel can be used to construct families of covariance functions based on the one-dimensional Wasserstein distance, see ?.

In general dimension, however, there is no indication that the function  $(\mu, \nu) \rightarrow W_2^2(\mu, \nu)$  defines a negative definite kernel. Hence, since the set of measures on  $\mathbb{R}^p$  is a manifold endowed with the Monge-Kantorovich (Wasserstein) distance, we suggest to compare the distributions  $\mu$  and  $\nu$  around a central measure. This point of view is similar to what has been proposed in ? for image analysis. For this, we propose to consider that the distributions of interest are realizations of a distribution over the set of distributions. Then, we construct a covariance kernel by using the barycenter of this distribution (over distributions), and by using optimal transport maps. The following section is devoted to the construction of the so-called Wasserstein barycenter.

## 2.2. Barycenters of distributions

Let us consider the set  $\mathcal{W}_2(\mathbb{R}^p)$  of probability measures on  $\mathbb{R}^p$  with finite moments of order two. For two  $\mu, \nu$  in  $\mathcal{W}_2(\mathbb{R}^p)$ , we denote by  $\Pi(\mu, \nu)$  the set of all probability measures  $\pi$  over the product set  $\mathbb{R}^p \times \mathbb{R}^p$  with first (resp. second) marginal  $\mu$  (resp.  $\nu$ ).

The transportation cost with quadratic cost function, or quadratic transportation cost, between these two measures  $\mu$  and  $\nu$  is defined as

$$\mathcal{T}_2(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int \|x - y\|^2 d\pi(x, y). \quad (4)$$

This transportation cost allows to endow the set  $\mathcal{W}_2(\mathbb{R}^p)$  with a metric by defining the quadratic Monge-Kantorovich, or quadratic Wasserstein distance between  $\mu$  and  $\nu$  as

$$W_2(\mu, \nu) = \mathcal{T}_2(\mu, \nu)^{1/2}. \quad (5)$$

A probability measure  $\pi$  in  $\Pi(\mu, \nu)$  realizing the infimum in (4) is called an optimal coupling. This vocabulary transfers to a random vector  $(X_1, X_2)$  with distribution  $\pi$ .

When dealing with a collection of distributions  $\mu_1, \dots, \mu_n$ , we can define a notion of variation of these distributions. For any  $\nu \in \mathcal{W}_2(\mathbb{R}^p)$ , set

$$\text{Var}(\nu) = \sum_{i=1}^n W_2^2(\nu, \mu_i).$$

Finding the distribution minimizing the variance of the distributions has been tackled when defining the notion of barycenter of distributions with respect to Wasserstein's distance in the seminal work of ?. More precisely, given  $p \geq 1$ , they provide conditions to ensure existence and uniqueness of the barycenter of the probability measures  $(\mu_i)_{1 \leq i \leq n}$  with weights  $(\lambda_i)_{1 \leq i \leq n}$ , i.e. a minimizer of the following criterion

$$\nu \mapsto \sum_{i=1}^n \lambda_i W_2^2(\nu, \mu_i). \quad (6)$$

Along the last two years several works have studied empirical properties of the barycenters and their applications to several fields. We refer for instance to ?, ? and references therein. Hence the Wasserstein barycenter or Fréchet mean of distribution appears to be a meaningful feature to represent the mean variations of a set of distributions.

This notion of Wasserstein barycenter has been recently extended to distributions defined on  $\mathcal{W}_2(\mathcal{W}_2(\mathbb{R}^p))$ . Let  $\mathbb{P}$  be a distribution in  $\mathcal{W}_2(\mathcal{W}_2(\mathbb{R}^p))$  and consider  $\mu_1, \dots, \mu_n$  i.i.d probabilities drawn according to the distribution  $\mathbb{P}$ . In this framework, the Wasserstein distance between distributions on  $\mathcal{W}_2(\mathbb{R}^p)$  is defined, for any  $\nu \in \mathcal{W}_2(\mathbb{R}^p)$ , as

$$W_2^2(\mathbb{P}, \delta_\nu) = \int W_2^2(\nu, \mu) d\mathbb{P}(\mu). \quad (7)$$

If  $\tilde{\mu}$  is a random distribution with distribution  $\mathbb{P}$  this corresponds to

$$W_2^2(\mathbb{P}, \delta_\nu) = \mathbb{E}_{\{\tilde{\mu} \sim \mathbb{P}\}} W_2^2(\tilde{\mu}, \nu).$$

Note that we will use the same notations for the Wasserstein distances over distributions in  $\mathcal{W}_2(\mathbb{R}^p)$  and over distributions on distributions in  $\mathcal{W}_2(\mathcal{W}_2(\mathbb{R}^p))$ . The space  $\mathcal{W}_2(\mathcal{W}_2(\mathbb{R}^p))$  inherits the properties of the space  $\mathcal{W}_2(\mathbb{R}^p)$  and is the good space to generalize the asymptotic properties of sequences of Wasserstein barycenters.

Actually, we define as a Wasserstein barycenter of  $\mathbb{P}$ , a probability  $\bar{\mu}$  in  $\mathcal{W}_2(\mathbb{R}^p)$  such that, if it exists,

$$\int W_2^2(\bar{\mu}, \mu) d\mathbb{P}(\mu) = \inf \left\{ \int W_2^2(\nu, \mu) d\mathbb{P}(\mu), \nu \in \mathcal{W}_2(\mathbb{R}^p) \right\}.$$

First, we point out that the notion of barycenter developed in (6) corresponds also to the barycenter of the atomic probability  $\mathbb{P}$  on the Wasserstein space, defined by

$$\mathbb{P} = \sum_{i=1}^n \lambda_i \delta_{\mu_i}.$$

Then, we recall the following theorem from ? following ? that guarantees the existence and uniqueness of this barycenter under some assumptions.

**Theorem 1 (Existence of a Wasserstein Barycenter)** *Let  $\mathbb{P} \in \mathcal{W}_2(\mathcal{W}_2(\mathbb{R}^p))$ . Assume that every distribution in the support of  $\mathbb{P}$  is absolutely continuous with respect to Lebesgue measure on  $\mathbb{R}^p$ . Then there exists a unique distribution  $\bar{\mu} \in \mathcal{P}$  defined as*

$$\bar{\mu} = \arg \min_{\nu \in \mathcal{W}_2(\mathbb{R}^p)} \left\{ \int W_2^2(\nu, \mu) d\mathbb{P}(\mu) \right\}. \quad (8)$$

Using the expression (7), we can see that Theorem 1 can be reformulated as stating the existence of the metric projection of  $\mathbb{P}$  onto the subset of  $\mathcal{W}_2(\mathcal{W}_2(\mathbb{R}^p))$  composed of Dirac measures.

Consider a sample of i.i.d random distributions  $\mu_i, i = 1, \dots, n$  drawn with distribution  $\mathbb{P}$  and set  $\bar{\mu}$  its barycenter. Let for fixed  $n, \bar{\mu}_n$  be the empirical barycenter of the  $\mu_1, \dots, \mu_n$ , defined as

$$\sum_{i=1}^n \lambda_i W_2^2(\bar{\mu}_n, \mu_i) = \inf \left\{ \sum_{i=1}^n \lambda_i W_2^2(\nu, \mu_i), \nu \in \mathcal{W}_2(\mathbb{R}^p), \right\}$$

with  $\lambda_1 = \dots = \lambda_n = 1$ . This empirical barycenter exists and is unique as soon as one of the  $\mu_i$  is absolutely continuous w.r.t Lebesgue measure in  $\mathbb{R}^p$ .

The following theorem states that under uniqueness assumption the empirical Wasserstein barycenter  $\bar{\mu}_n$  converges to the population Wasserstein barycenter  $\bar{\mu}$ .

**Theorem 2** *Assume that  $\mathbb{P}$  belongs to  $\mathcal{W}_2(\mathcal{W}_2(\mathbb{R}^p))$  and that its barycenter is unique. Let  $\mu_1, \dots, \mu_n$  be independently drawn from  $\mathbb{P}$  and let  $\bar{\mu}_n$  be defined as above. Then the empirical barycenter  $\bar{\mu}_n$  is consistent in the sense that when  $n$  goes to infinity we have*

$$W_2(\bar{\mu}, \bar{\mu}_n) \longrightarrow 0, \text{ (a.s.)}$$

Hence when considering random distributions drawn from a probability  $\mathbb{P}$ , the barycenter  $\mu$  enjoys some stability properties. Moreover it can be consistently estimated by its empirical counterpart. This provides a framework to build a kernel for Gaussian Processes indexed by distributions.

### 3. Construction of a kernel on multidimensional distributions

Let  $\mathbb{P} \in \mathcal{W}_2(\mathcal{W}_2(\mathbb{R}^p))$  satisfies the condition of Theorem 1. Consider a sample of i.i.d distributions  $\mu_i, i = 1, \dots, n$  drawn with distribution  $\mathbb{P}$  and set  $\bar{\mu}$  the barycenter of  $\mathbb{P}$ . Let for fixed  $n, \bar{\mu}_n$  be the empirical barycenter of the  $\mu_1, \dots, \mu_n$ , defined as in Section 2.2. The main idea consists in using optimal transportation maps to quantify the correlations between the observation of the process, that is to say to define a covariance kernel based on the Wasserstein distance.

For  $\mu \in \mathcal{W}_2(\mathbb{R}^p)$ , let  $T_\mu, T_{\mu,n} : \mathbb{R}^p \rightarrow \mathbb{R}^p$  be the optimal transportation maps defined by

$$T_{\mu\#}\mu = \bar{\mu}, \quad T_{\mu,n\#}\mu = \bar{\mu}_n,$$

where  $f_{\#}\pi = \pi \circ f^{-1}$  is the push-forward measure of a function  $f$  from a measure  $\pi$ , and

$$\|\text{id} - T_\mu\|_{L^2(\mu)} = W_2(\mu, \bar{\mu}), \quad \|\text{id} - T_{\mu,n}\|_{L^2(\mu)} = W_2(\mu, \bar{\mu}_n).$$

Let also, for  $i = 1, \dots, n$   $T_i = T_{\mu_i}$  and  $T_{i,n} = T_{\mu_i,n}$ .

Note that the maps  $T_\mu$  and  $T_{\mu,n}$  are uniquely defined when  $\mu$  is absolutely continuous w.r.t. Lebesgue measure. Indeed, because of the assumption on  $\mathbb{P}$ , both the barycenter and the empirical barycenter are absolutely continuous w.r.t Lebesgue measure on  $\mathbb{R}^p$ . Similarly,  $T_1, \dots, T_n$  and  $T_{1,n}, \dots, T_{n,n}$  are uniquely defined.

We point out that the existence of transportation maps that can be considered as gradients of convex functions is commonly referred to as Brenier's theorem and originated from Y. Brenier's work in the analysis and mechanics literature in ?. Much of the current interest in transportation problems emanates from this area of mathematics. We conform to the common use of the name. However, it is worthwhile pointing out that a similar statement was established earlier independently in a probabilistic framework in ? : they show existence of an optimal transport map for quadratic cost over Euclidean and Hilbert spaces, and prove monotonicity of the optimal map in some sense (Zarantarello monotonicity).

We will construct a valid kernel using the maps  $T_\mu^{-1}$ , on the Hilbert space  $L^2(\bar{\mu})$ , for absolutely continuous distributions  $\mu$ .

In the following, we provide a generic way to construct this type of functional covariance functions. Consider a continuous function  $F : \mathbb{R}^+ \rightarrow \mathbb{R}$ , so that, for any  $d \in \mathbb{N}$ , the function

$$K := \mathbb{C}^d \times \mathbb{C}^d \mapsto \mathbb{R}$$

$$(u, v) \rightarrow K(u, v) = F(\|u - v\|^2),$$

is a positive definite kernel. Then consider the following function  $K$  on  $\mathcal{W}_2(\mathbb{R}^p) \times \mathcal{W}_2(\mathbb{R}^p)$  defined by

$$K(\mu, \nu) = F(\|T_\mu^{-1} - T_\nu^{-1}\|_{L^2(\bar{\mu})}^2), \quad (9)$$

where  $\bar{\mu}$  is the barycenter of  $\mathbb{P}$  defined in Theorem 1.

**Theorem 3** *The kernel defined in (9) is a covariance kernel over absolutely continuous distributions in  $\mathcal{W}_2(\mathbb{R}^p)$ .*

The proof relies on the following Proposition which provides a generic way of constructing covariance kernels on an Hilbert space provided we have covariance kernels on  $\mathbb{C}^d \times \mathbb{C}^d$  for any  $d \in \mathbb{N}$ . Applied with  $H = L^2(\bar{\mu})$ , it proves the previous theorem.

**Proposition 1 (Validity of Covariance on distributions)** *Let  $F : \mathbb{R}^+ \rightarrow \mathbb{R}$  be such that, for any  $d \in \mathbb{N}$ , the function  $K : \mathbb{C}^d \times \mathbb{C}^d \rightarrow \mathbb{R}$  defined by  $K(u, v) = F(\|u - v\|)$  is non-negative definite. Let  $K_H$  be the function defined on an Hilbert space  $H$  with norm  $\|\cdot\|_H$  as, for all  $(f, g) \in H^2$ ,  $K_H(f, g) = F(\|f - g\|_H)$ . Then  $K_H$  is non-negative definite.*

*Furthermore, assume that for any  $d \in \mathbb{N}$  and for any pairwise different  $u_1, \dots, u_n \in \mathbb{C}^d$ , the matrix  $(F(\|u_i - u_j\|))_{\{i,j\}}$  is invertible. Then for pairwise distinct  $f_1, \dots, f_n$  in  $H$ , the matrix  $(K_H(f_i, f_j))_{\{i,j\}}$  is invertible.*

The previous Proposition provides a generic way of construction covariance or kernels on Hilbert spaces provided we have a valid covariance model on  $\mathbb{C}^d \times \mathbb{C}^d$ .

When  $\mathbb{P}$  is not observed, we are only given the sample of random distributions. Hence only the empirical version  $\mathbb{P}_n = \frac{1}{n} \sum_{i=1}^n \delta_{\mu_i}$  is available. Hence, we need to approximate the barycenter  $\bar{\mu}$  by its empirical counterpart  $\bar{\mu}_n$ . Let, for a function  $F$  satisfying the condition of Proposition 1,

$$K_n(\mu, \nu) = F(\|T_{\mu,n}^{-1} - T_{\nu,n}^{-1}\|_{L^2(\bar{\mu}_n)}^2),$$

be the empirical kernel. We want to prove that this empirical kernel provides a good approximation of the valid covariance kernel  $K$ . Actually, using the consistency property of Theorem 2, the empirical barycenter is a consistent estimate for  $\bar{\mu}$ . Hence we can show that the empirical covariance kernel converges to the true covariance kernel.

**Proposition 2 (Consistency of Kernel)** *Let  $F$  in (9) be continuous. This empirical kernel is a good approximation of the true covariance kernel in the sense that, for any two fixed absolutely continuous measures  $\mu$  and  $\nu$  in  $\mathcal{W}_2(\mathbb{R}^p)$ , we have*

$$K_n(\mu, \nu) \rightarrow K(\mu, \nu)$$

*a.s. when  $n$  goes to infinity.*

**Proof** Using the continuity of the function  $F$ , it is enough to show that a.s.

$$\|T_{\mu,n}^{-1} - T_{\nu,n}^{-1}\|_{L^2(\mu_n)}^2 - \|T_{\mu}^{-1} - T_{\nu}^{-1}\|_{L^2(\bar{\mu})}^2 \rightarrow 0.$$

Lemma 7, whose proof is presented in the Appendix, leads to the result. ■

In the next Corollary, we show that the consistency result in Proposition 2 implies that the conditional means and variances based on the empirical kernel asymptotically coincide with those based on the true kernel.

**Corollary 4** *Let  $N \in \mathbb{N}$  and let  $\mu_1, \dots, \mu_N, \mu$  be fixed absolutely continuous measures in  $\mathcal{W}_2(\mathbb{R}^p)$ . Let  $y = (y_1, \dots, y_N)^\top$  be fixed in  $\mathbb{R}^N$ . Set  $R = [K(\mu_i, \mu_j)]_{1 \leq i, j \leq N}$  and assume that  $R$  is invertible. Let  $Y$  be a Gaussian process with zero mean function and covariance function given by (9). Then*

$$\mathbb{E}(Y_\mu | Y_{\mu_1} = y_1, \dots, Y_{\mu_N} = y_N) = r_\mu^\top R^{-1} y$$

*with  $r_\mu = (K(\mu, \mu_1), \dots, K(\mu, \mu_N))^\top$ . Let*

$$\mathbb{E}_n(Y_\mu | Y_{\mu_1}, \dots, Y_{\mu_N}) = r_{\mu,n}^\top R_n^{-1} y$$

*with  $r_{\mu,n} = (K_n(\mu, \mu_1), \dots, K_n(\mu, \mu_N))^\top$  and  $R_n = [K_n(\mu_i, \mu_j)]_{1 \leq i, j \leq N}$ . Also*

$$\text{Var}(Y_\mu | Y_{\mu_1} = y_1, \dots, Y_{\mu_N} = y_N) = K(\mu, \mu) - r_\mu^\top R^{-1} r_\mu$$

*and we let*

$$\text{Var}_n(Y_\mu | Y_{\mu_1}, \dots, Y_{\mu_N}) = K_n(\mu, \mu) - r_{\mu,n}^\top R_n^{-1} r_{\mu,n}.$$

*Then, a.s. as  $n \rightarrow \infty$ ,*

$$\begin{aligned} \mathbb{E}_n(Y_\mu | Y_{\mu_1}, \dots, Y_{\mu_N}) &\rightarrow \mathbb{E}(Y_\mu | Y_{\mu_1}, \dots, Y_{\mu_N}) \\ \text{and } \text{Var}_n(Y_\mu | Y_{\mu_1}, \dots, Y_{\mu_N}) &\rightarrow \text{Var}(Y_\mu | Y_{\mu_1}, \dots, Y_{\mu_N}). \end{aligned}$$

**Proof** The Corollary is a direct consequence of the facts that  $N$  is fixed as  $n \rightarrow \infty$  and that  $R$  is invertible.  $\blacksquare$

Finally, let us give an example of covariance kernels on  $\mathcal{W}_2(\mathbb{R}^p)$  obtained from our construction. For any  $\sigma^2 > 0, \ell > 0, s \in [0, 2]$  the function  $\mathbb{R}^+ \rightarrow \mathbb{R}$  defined by

$$F_\theta(x) := \sigma^2 \exp(-(x/\ell)^s), \quad \theta := (\sigma, \ell, s),$$

satisfies the condition of Proposition 1 (see e.g. ?). Hence, the function  $K$  defined by

$$K_\theta(\mu, \nu) := \sigma^2 \exp\left(-\left[\|T_\mu^{-1} - T_\nu^{-1}\|_{L^2(\bar{\mu})}/\ell\right]^s\right)$$

is a covariance kernel on  $\mathcal{W}_2(\mathbb{R}^p)$ . Other examples can be obtained from the Matérn covariance function ?.

Note that when considering a kernel  $K$ , a natural property to be studied would be its universality. Actually, a kernel is said to be universal on  $\Omega \subset \mathcal{W}(\mathbb{R}^p)$  as soon as the space generated by its linear combinations  $\mu \in \mathcal{W}(\Omega) \mapsto \sum_{i=1}^n \alpha_i K(\mu, \mu_i) \in \mathbb{R}$  can generate all continuous functions on  $\mathcal{W}(\Omega)$ . The general form (9) of the kernel may provide uniform kernels under regularity assumptions on the transportation maps  $T_i$ . More precisely injectivity and continuity are required as pointed out in ? to get a universal kernel. Yet regularity of transportation maps in general dimensions is a difficult issue that has received a lot of attention in the last years see for instance to ? and such conditions can not be guaranteed in a very general framework but could only be studied for very particular class of distributions, leading to too restrictive cases, which are not at the heart of this paper.

## 4. Asymptotic Properties

### 4.1. Gaussian processes on Hilbert spaces

In this section, we consider a parametric set of covariance functions on balls of Wasserstein space, namely  $\mathcal{B}_{2,L,\bar{\mu}}(\mathbb{R}^p)$  where  $\mathcal{B}_{2,L,\bar{\mu}}(\mathbb{R}^p) = \{\mu \in \mathcal{W}_2(\mathbb{R}^p); W_2(\mu, \bar{\mu}) \leq L\}$  for a fixed  $L < \infty$  and for  $\bar{\mu}$  as in Section 3. This parametric set is  $\{K_\theta; \theta \in \Theta\}$ , with  $\Theta \subset \mathbb{R}^q$  for  $q \in \mathbb{N}$  and where for all  $\theta \in \Theta$ ,  $K_\theta$  is a positive definite kernel on  $\mathcal{B}_{2,L,\bar{\mu}}(\mathbb{R}^p)$ . We further consider that for any  $\theta \in \Theta$ , for any  $\mu, \nu \in \mathcal{B}_{2,L,\bar{\mu}}(\mathbb{R}^p)$ , we have

$$K_\theta(\mu, \nu) = F_\theta(\|T_\mu^{-1} - T_\nu^{-1}\|_{L^2(\bar{\mu})}^2), \quad (10)$$

with the notation of Section 3. We assume also that  $F_\theta$  satisfies the condition of Proposition 1 for all  $\theta \in \Theta$ .

Hence, for  $\theta \in \Theta$ ,  $K_\theta$  is the covariance function of a Gaussian process defined on

$$\bar{\mathcal{B}}_{2,L,\bar{\mu}} = \{f \in L^2(\bar{\mu}), \|f - \text{id}\|_{L^2(\bar{\mu})} \leq T\}.$$

The space  $\bar{\mathcal{B}}_{2,L,\bar{\mu}}$  is a bounded subset of a Hilbert space with an infinite countable basis. Hence, in the rest of the section, we study some asymptotic properties of Gaussian processes indexed by a bounded subset of an Hilbert space.

## 4.2. Microergodic covariance parameters

Let  $\mathcal{H}$  be a Hilbert space with an infinite countable basis  $(h_i)_{i \in \mathbb{N}}$ . Let  $h_0 \in \mathcal{H}$  be fixed and let  $\bar{\mathcal{B}}_{2,L} = \{h \in \mathcal{H}; \|h - h_0\|_{\mathcal{H}} \leq L\}$ . Let  $\bar{F} = \mathbb{R}^{\bar{\mathcal{B}}_{2,L}}$  be the set of functions from  $\bar{\mathcal{B}}_{2,L}$  to  $\mathbb{R}$ . Let  $\mathcal{F}$  be the cylinder sigma algebra on  $\bar{F}$  generated by the functions  $f \rightarrow (f(h_1), \dots, f(h_r))$  for any  $r \in \mathbb{N}$  and  $h_1, \dots, h_r \in \mathcal{H}$ . For any  $\theta \in \Theta$ , let  $\mathbb{P}_{\theta}$  be the measure on  $(\bar{F}, \mathcal{F})$  equal to the law of a Gaussian process on  $\bar{\mathcal{B}}_{2,L}$  with mean function zero and covariance function  $(h_1, h_2) \rightarrow F_{\theta}(\|h_1 - h_2\|_{\mathcal{H}})$ . Then, following ?, we say that the covariance parameter  $\theta$  is microergodic if, for any  $\theta_1, \theta_2 \in \Theta$  with  $\theta_1 \neq \theta_2$ , the measures  $\mathbb{P}_{\theta_1}$  and  $\mathbb{P}_{\theta_2}$  are orthogonal, that is there exists  $\mathcal{A} \in \mathcal{F}$  so that  $\mathbb{P}_{\theta_1}(\mathcal{A}) = 1$  and  $\mathbb{P}_{\theta_2}(\mathcal{A}) = 0$ .

For Gaussian processes indexed by a fixed bounded subset of  $\mathbb{R}^d$ , for  $d \in \mathbb{N}$ , microergodicity is an important concept. Indeed, it is a necessary condition for consistent estimators of  $\theta$  to exist under fixed-domain asymptotics ?, and a fair amount of work has been devoted to showing microergodicity or non-microergodicity of parameters, for various models of covariance functions ????. In this section, we extend these types of results to Gaussian processes indexed by a bounded subset of  $\mathcal{H}$ .

## 4.3. A general microergodicity result

In the next theorem, we show that, under very mild assumptions, the covariance parameter  $\theta$  is microergodic in our setting.

**Theorem 5** *Assume that there does not exist  $\theta_1, \theta_2 \in \Theta$ , with  $\theta_1 \neq \theta_2$ , so that  $t \rightarrow F_{\theta_1}(t) - F_{\theta_2}(t)$  is constant on  $[0, 2L]$ . Then the covariance parameter  $\theta$  is microergodic.*

In Theorem 5, the condition on the parametric family  $\{F_{\theta}; \theta \in \Theta\}$  holds for all the commonly used families of covariance functions which are used when applied to norms of differences of vectors in  $\mathbb{R}^d$ . These commonly used families include notably the Matérn covariance functions, the generalized Wendland covariance functions, the spherical covariance functions and the power exponential covariance functions ????. Hence, Theorem 5 shows that it is possible that consistent estimators exist for  $\theta$ , in many parametric models of covariance functions of the form (10).

Finally, consider a family of covariance functions  $\{\tilde{K}_{\theta}; \theta \in \Theta\}$  on  $\mathbb{R}^d$  satisfying  $\tilde{K}_{\theta}(x_1, x_2) = F_{\theta}(\|x_1 - x_2\|)$  with  $F_{\theta}$  satisfying the assumption of Theorem 5 and with  $\|\cdot\|$  the Euclidean norm. Then, one can see that if  $\theta$  is microergodic for  $d_1 \in \mathbb{N}$ , it is also microergodic for any  $d_2 \geq d_1$  (see also ?). That is, an higher dimension of the input space yields more microergodicity. In agreement with this fact, Theorem 5 can be interpreted as follows: when  $d$  is infinite, the covariance parameter  $\theta$  is always microergodic.

## 5. Computation aspects and an illustration

In practice, computing optimal transportation maps is a difficult issue in the general case, especially when the dimension of the problem increases.

A first solution consists, in many cases in approximating it by an empirical counterpart. Let  $\mu_p$  and  $\nu_p$  be empirical measures sampled from  $\mu$  and  $\nu$  respectively. Then the optimal Monge map  $T_{\#} \mu = \nu$  can be replaced by  $T_{\#}^p \mu_p = \nu_p$ , see e.g. ? (Theorem A.1). In this case problem of finding  $T^p$  is reduced to the solution of assignment problem with quadratic cost and can be solved by *adagio* R-package by ?.

In some special cases, the optimal transportation maps can be written down explicitly only for some particular class of admissible transformations. An example of explicit calculations is given by a family of Gaussian distribution. Consider a distribution over some subset of covariance matrices  $\mathbb{P}_S$ , which generates the unique population barycenter  $\bar{\mu} = \mathcal{N}(0, \bar{S})$ .

Let  $\{\mu_i\}_{i=1,\dots,n}$  be a family of observed random Gaussian distributions with zero mean and non-degenerated covariance  $S_i$ :  $\mu_i = \mathcal{N}(0, S_i)$ ,  $S_i \sim \mathbb{P}_S$ . An empirical barycenter is recovered uniquely:  $\bar{\mu}_n = \mathcal{N}(0, \bar{S}_n)$  with  $\bar{S}_n$  a solution of the following fixed-point equation  $\bar{S}_n = \frac{1}{n} \sum (S_i^{1/2} \bar{S}_n S_i^{1/2})^{1/2}$ . This result is well known and has been described in many paper, see for instance in the seminal work ?. The solution can be obtained by an iterative method, presented in ?.

The setting allows to write down an optimal transport plan between  $T_i$  between  $\mu_i$  and  $\bar{\mu}$  and its inverse explicitly:

$$T_i = S_i^{-1/2} (S_i^{1/2} \bar{S} S_i^{1/2})^{1/2} S_i^{-1/2}, \quad T_i^{-1} = \bar{S}^{-1/2} (\bar{S}^{1/2} S_i \bar{S}^{1/2})^{1/2} \bar{S}^{-1/2}.$$

In this case, we can compute the distance between the transport plans in  $L^2(\bar{\mu})$  using the expression in (5)  $\|T_i^{-1} - T_j^{-1}\|_{L^2(\bar{\mu})}^2$ , as the distance is the variance of a linear transform of Gaussian random variable:

$$\|T_i^{-1} - T_j^{-1}\|_{L^2(\bar{\mu})}^2 = \left\| \bar{S}^{-1/2} \left[ (\bar{S}^{1/2} S_i \bar{S}^{1/2})^{1/2} - (\bar{S}^{1/2} S_j \bar{S}^{1/2})^{1/2} \right] \right\|_F^2.$$

The same expression holds for  $\|T_{i,n}^{-1} - T_{j,n}^{-1}\|_{L^2(\bar{\mu})}^2$ . We can see that in this case the kernel amounts to compute a natural distance between the two distributions  $\mu_i$  and  $\mu_j$  obtained by the scale deformation  $S_i^{1/2} X$  and  $S_j^{1/2} X$  of a Gaussian random variable  $X \sim \mathcal{N}(0, Id)$ . This distance is then used through any kernel which provides some insights on a proper notion of covariance between processes indexed by these two distributions.

In what follows we present some simulations to highlight the consistency of the empirical kernel we simulated. For this we generate covariance matrices  $S_i$  as  $S_i = A_i A_i'$ , where  $A_i = (a_{jk})_{j,k=1}^d$ ,  $a_{jk} \sim \text{Unif}[5, 15]$ . Fig. 1 illustrates Proposition 2 for Gaussian distributions on  $\mathbb{R}^d$ ,  $d \in \{4, 7, 15, 30\}$  while Table 1 provides the estimation error.

Table 1: Error

	n = 20	n = 140	n = 260	n = 380	n = 500	n = 620
d = 4	1.52	0.69	0.16	0.29	0.24	0.14
d = 7	2.08	0.59	0.17	0.19	0.11	0.14
d = 15	0.91	0.12	0.09	0.08	0.05	0.05
d = 30	0.90	0.13	0.05	0.03	0.04	0.02

## 6. Conclusion and Future Directions

In this work, we have provided a theoretical way to use Wasserstein barycenters in order to define general kernels using optimal transportation maps. Considering the distance between the optimal transportation maps provide a natural way to quantify correlations between the values of a process

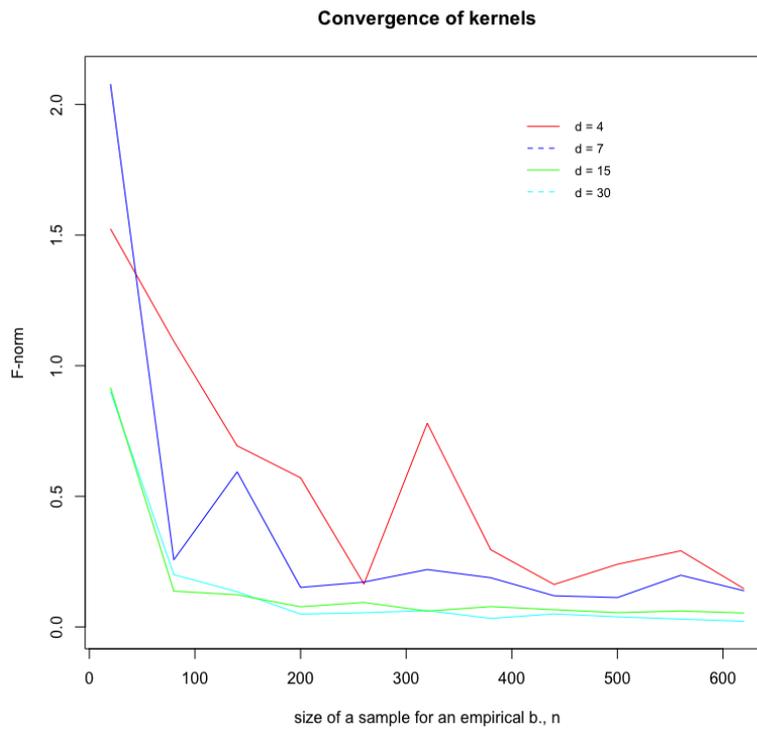


Figure 1: Convergence of kernels

indexed by the distribution and provides a generalization to multi-dimensional case of the work in ?. Using barycenter requires that the distributions are drawn according to the same measure over the set of distributions. This restricts the framework of the study to the case where the Gaussian process is defined on the support of this measure. For applications, this does not play a too important feature since inputs are often simulated according to a specified distribution. Yet for theoretical issues, this sets the frame of this study to the infill case and not the asymptotic frame. In this case, few results exist in the statistical literature on Kriging, and thus we focused on micro-ergodicity of the parameters, proving that consistent estimate can be studied.

Finally contrary to the one-dimensional case, computational issues arise naturally when the Wasserstein distance is required. Hence the computation of a barycenter with respect to Wasserstein distance is a difficult optimization program, unless the distributions are Gaussian, leading to tractable computations as shown in Section 5 . Yet this idea of linearization around the barycenter to obtain a valide covariance kernel could be used and generalized to regularized Wasserstein distance using methods proposed in ? for instance to provide a more tractable way of building kernels.

## Appendix A. Proofs

### Proof of Proposition 1

**Proof** Let  $f_1, \dots, f_n$  in  $H$  and consider the matrix  $\tilde{C} = (\langle f_i, f_j \rangle_H)_{\{i,j\}}$ . This matrix is a Gramian matrix in  $\mathbb{R}^{n \times n}$  hence there exists a non negative diagonal matrix  $D$  and an orthogonal matrix  $P$  such that

$$\tilde{C} = PDP' = PD^{1/2}D^{1/2}P'.$$

Let  $e_1, \dots, e_n$  be the canonical basis of  $\mathbb{R}^n$ . Then

$$e_i \tilde{C} e_j' = u_i u_j'$$

where  $u_i = e_i P D^{1/2}$ . Note that the  $u_i$ 's are vectors in  $\mathbb{C}^n$  that depend on the  $f_1, \dots, f_n$ . Hence we get that

$$\langle f_i, f_j \rangle_H = \langle u_i, u_j \rangle$$

where  $\langle, \rangle$  denotes the usual scalar product on  $\mathbb{C}^n$ . Hence we get that for any functions  $f_1, \dots, f_n$  in  $H$  there are  $u_1, \dots, u_n$  in  $\mathbb{C}^n$  such that  $\|f_i - f_j\|_H = \|u_i - u_j\|$ . So any covariance matrix that can be written as  $[F(\|f_i - g_j\|_H)]_{i,j}$  can be seen as a covariance matrix  $[F(\|u_i - u_j\|)]_{i,j}$  on  $\mathbb{C}^n$  and inherits its properties. The invertibility and non-negativity of this covariance matrix entail the invertibility and non-negativity of the first one, which proves the result. ■

### Proof of Proposition 2

Recall that the empirical barcyenters  $(\bar{\mu}_n)_n$  is a sequence of continuous measures converging to  $\bar{\mu}$  in 2-Wasserstein distance:  $W_2(\bar{\mu}_n, \bar{\mu}) \rightarrow 0$  as  $n \rightarrow \infty$  and  $R_{n\#}\bar{\mu} = \bar{\mu}_n$  with  $W_2^2(\bar{\mu}, \bar{\mu}_n) = \|R_n\|_{L^2(\bar{\mu})}$ .

**Lemma 6** Fix some distribution  $\nu$  absolutely continous with respect to Lebesgue measure and let  $T = T_\nu$  and  $T_n = T_{\nu,n}$ . Then it holds a.s.

$$\|T - T_n\|_{L^2(\nu)}^2 \longrightarrow 0, \text{ as } n \rightarrow \infty.$$

**Proof** Fix  $n$  s.t.  $W_2(\bar{\mu}_n, \bar{\mu}) = \varepsilon_n$ . Consider  $\|\text{id} - R_n \circ T\|_{L^2(\nu)}$ . By change of variables and triangle inequality one obtains

$$\begin{aligned} \|\text{id} - R_n \circ T\|_{L^2(\nu)} &= \|T^{-1} - R_n\|_{L^2(\bar{\mu})} \leq \|T^{-1} - \text{id}\|_{L^2(\bar{\mu})} + \|R_n - \text{id}\|_{L^2(\bar{\mu})} \\ &\leq W_2(\nu, \bar{\mu}) + \varepsilon_n \leq W_2(\nu, \bar{\mu}_n) + 2\varepsilon_n. \end{aligned}$$

Since  $T_n$  is the optimal transport map from  $\nu$  to  $\mu_n$  we recall that  $W_2(\nu, \bar{\mu}_n) = \|\text{id} - T_n\|_{L^2(\nu)}$ . So due to the arbitrary choice of  $n$  it follows

$$\left| \|\text{id} - R_n \circ T\|_{L^2(\nu)} - \|\text{id} - T_n\|_{L^2(\nu)} \right| \xrightarrow{n \rightarrow \infty} 0. \quad (11)$$

Now we are ready to prove, that  $\|T_n - T\|_{L^2(\nu)} \xrightarrow{n \rightarrow \infty} 0$ . Assume the claim is wrong. Assume the claim is wrong:

$$T_n \xrightarrow{n \rightarrow \infty} T_1, \quad R_n \circ T \xrightarrow{n \rightarrow \infty} T_2, \quad \|T_1 - T_2\| > \varepsilon.$$

Thus

$$\|\text{id} - T_n\|_{L^2(\nu)} \xrightarrow{n \rightarrow \infty} \|\text{id} - T_1\|_{L^2(\nu)}, \quad \|\text{id} - R_n \circ T\|_{L^2(\nu)} \xrightarrow{n \rightarrow \infty} \|\text{id} - T_2\|_{L^2(\nu)},$$

which contradicts to (11) ■

The next lemma is a key ingredient in the proof of the fact that the true kernel can be replaced by its empirical counterpart.

**Lemma 7** Consider two fixed absolutely continuous measures  $\mu$  and  $\nu$  in  $\mathcal{W}_2(\mathbb{R}^p)$ . We have a.s.

$$\left| \|T_\mu^{-1} - T_\nu^{-1}\|_{L^2(\bar{\mu})}^2 - \|T_{\mu,n}^{-1} - T_{\nu,n}^{-1}\|_{L^2(\bar{\mu}_n)}^2 \right| \rightarrow 0, \text{ as } n \rightarrow \infty.$$

**Proof** Consider  $\|T_{\mu,n}^{-1} - T_{\nu,n}^{-1}\|_{L^2(\bar{\mu}_n)}$ . Change of variables and triangle inequality yield

$$\begin{aligned} \|T_{\mu,n}^{-1} - T_{\nu,n}^{-1}\|_{L^2(\bar{\mu}_n)} &= \|T_{\mu,n}^{-1} \circ R_n - T_{\nu,n}^{-1} \circ R_n\|_{L^2(\bar{\mu})} \\ &\leq \|T_{\mu,n}^{-1} \circ R_n - T_\mu^{-1}\|_{L^2(\bar{\mu})} + \|T_{\nu,n}^{-1} \circ R_n - T_\nu^{-1}\|_{L^2(\bar{\mu})} + \|T_\mu^{-1} - T_\nu^{-1}\|_{L^2(\bar{\mu})}. \end{aligned}$$

Therefore one obtains

$$\begin{aligned} &\|T_{\mu,n}^{-1} - T_{\nu,n}^{-1}\|_{L^2(\bar{\mu}_n)} - \|T_\mu^{-1} - T_\nu^{-1}\|_{L^2(\bar{\mu})} \\ &\leq \|T_{\mu,n}^{-1} \circ R_n - T_\mu^{-1}\|_{L^2(\bar{\mu})} + \|T_{\nu,n}^{-1} \circ R_n - T_\nu^{-1}\|_{L^2(\bar{\mu})} \xrightarrow{n \rightarrow \infty} 0 \end{aligned}$$

where the last relation holds due to Lemma 6. ■

### Proof of Proposition 5

**Proof** Without loss of generality, we can assume that  $h_0 = 0 \in \mathcal{H}$ . Let  $\theta_1, \theta_2 \in \Theta$ , with  $\theta_1 \neq \theta_2$ . Then, there exists  $t^* \in [0, L]$  so that  $F_{\theta_1}(0) - F_{\theta_1}(2t^*) \neq F_{\theta_2}(0) - F_{\theta_2}(2t^*)$ .

For any  $n \in \mathbb{N}$ , let  $e_1, \dots, e_n \in \mathcal{H}$  satisfy  $(e_i | e_j)_{\mathcal{H}} = \mathbf{1}_{i=j}$ . Consider the  $2n$  elements  $(f_1, \dots, f_{2n})$  made by the pairs  $(-t^* e_i, t^* e_i)$  for  $i = 1, \dots, n$ . Consider a Gaussian process  $Y$  on  $\overline{\mathcal{B}}_{2,L}$  with mean function zero and covariance function  $K_{\theta_1}$ . Then, the Gaussian vector  $Z = (Y(f_i))_{i=1, \dots, 2n}$  has covariance matrix  $C$  given by

$$C_{i,j} = \begin{cases} F_{\theta_1}(0) & \text{if } i = j \\ F_{\theta_1}(2t^*) & \text{if } i \text{ even and } j = i + 1 \\ F_{\theta_1}(2t^*) & \text{if } i \text{ odd and } j = i - 1 \\ F_{\theta_1}(\sqrt{2}t^*) & \text{else.} \end{cases}$$

Hence, we have  $C = D + M$  where  $M$  is the matrix with all components equal to  $K_{\theta_1}(\sqrt{2}t^*)$  and where  $D$  is block diagonal, composed of  $n$  blocks of size  $2 \times 2$ , with each block equal to

$$B_{2,2} = \begin{pmatrix} F_{\theta_1}(0) - F_{\theta_1}(\sqrt{2}t^*) & F_{\theta_1}(2t^*) - F_{\theta_1}(\sqrt{2}t^*) \\ F_{\theta_1}(2t^*) - F_{\theta_1}(\sqrt{2}t^*) & F_{\theta_1}(0) - F_{\theta_1}(\sqrt{2}t^*) \end{pmatrix}.$$

Hence, in distribution,  $Z = M + E$ , with  $M$  and  $E$  independent,  $M = (z, \dots, z)$  where  $z \sim \mathcal{N}(0, K_{\theta_1}(\sqrt{2}t^*))$  and where the  $n$  pairs  $(E_{2k+1}, E_{2k+2})$ ,  $k = 0, \dots, n-1$  are independent, with distribution  $\mathcal{N}(0, B_{2,2})$ . Hence, with  $\overline{Z}_1 = (1/n) \sum_{k=0}^{n-1} Z_{2k+1}$ ,  $\overline{Z}_2 = (1/n) \sum_{k=0}^{n-1} Z_{2k+2}$  and  $\overline{E} = (1/n) \sum_{k=0}^{n-1} (E_{2k+1}, E_{2k+2})^t$ , we have

$$\begin{aligned} \widehat{B} &:= \frac{1}{n} \sum_{i=0}^{n-1} \begin{pmatrix} Z_{2i+1} - \overline{Z}_1 \\ Z_{2i+2} - \overline{Z}_2 \end{pmatrix} \begin{pmatrix} Z_{2i+1} - \overline{Z}_1 \\ Z_{2i+2} - \overline{Z}_2 \end{pmatrix}^t \\ &= \frac{1}{n} \sum_{i=0}^{n-1} \begin{pmatrix} E_{2i+1} \\ E_{2i+2} \end{pmatrix} \begin{pmatrix} E_{2i+1} \\ E_{2i+2} \end{pmatrix}^t - \overline{E} \overline{E}^t \\ &\xrightarrow{p}_{n \rightarrow \infty} B_{2,2}. \end{aligned}$$

Hence, there exists a subsequence  $n' \rightarrow \infty$  so that, almost surely  $\widehat{B} \rightarrow B_{2,2}$  as  $n' \rightarrow \infty$ . Hence, almost surely  $\widehat{B}_{11} - \widehat{B}_{1,2} \rightarrow K_{\theta_1}(0) - K_{\theta_1}(2t^*)$  as  $n' \rightarrow \infty$ . Hence, the set

$$A = \left\{ g \in \overline{F}; \widehat{B}_{2,2}(g(f_1), \dots, g(f_{2n'})) \rightarrow_{n' \rightarrow \infty} F_{\theta_1}(0) - F_{\theta_1}(2t^*) \right\}$$

satisfies  $P_{\theta_1}(A) = 1$ . With the same arguments, we can show  $P_{\theta_2}(B) = 1$ , where

$$B = \left\{ g \in \overline{F}; \widehat{B}_{2,2}(g(f_1), \dots, g(f_{2n''})) \rightarrow_{n'' \rightarrow \infty} F_{\theta_2}(0) - F_{\theta_2}(2t^*) \right\}$$

where  $n''$  is a subsequence extracted from  $n'$ . Since  $A \cap B = \emptyset$ , it follows that  $P_{\theta_2}(A) = 0$ . Hence,  $\theta$  is microergodic. ■

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